



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:30 PM UTC

PDB ID : 6NOT / pdb_00006not
Title : Crystal structure of a full length elongation factor G (EF-G) from *Rickettsia prowazekii*
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2019-01-16
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

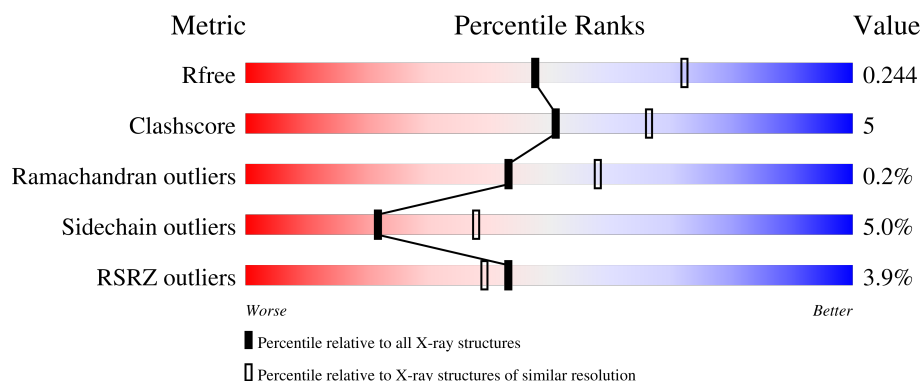
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	707	4% 79% 11% 10%
1	B	707	3% 74% 14% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9355 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	635	Total	C	N	O	S	0	0	0
			4679	2962	797	894	26			
1	B	631	Total	C	N	O	S	0	1	0
			4638	2941	791	879	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P41084
A	-6	ALA	-	expression tag	UNP P41084
A	-5	HIS	-	expression tag	UNP P41084
A	-4	HIS	-	expression tag	UNP P41084
A	-3	HIS	-	expression tag	UNP P41084
A	-2	HIS	-	expression tag	UNP P41084
A	-1	HIS	-	expression tag	UNP P41084
A	0	HIS	-	expression tag	UNP P41084
B	-7	MET	-	initiating methionine	UNP P41084
B	-6	ALA	-	expression tag	UNP P41084
B	-5	HIS	-	expression tag	UNP P41084
B	-4	HIS	-	expression tag	UNP P41084
B	-3	HIS	-	expression tag	UNP P41084
B	-2	HIS	-	expression tag	UNP P41084
B	-1	HIS	-	expression tag	UNP P41084
B	0	HIS	-	expression tag	UNP P41084

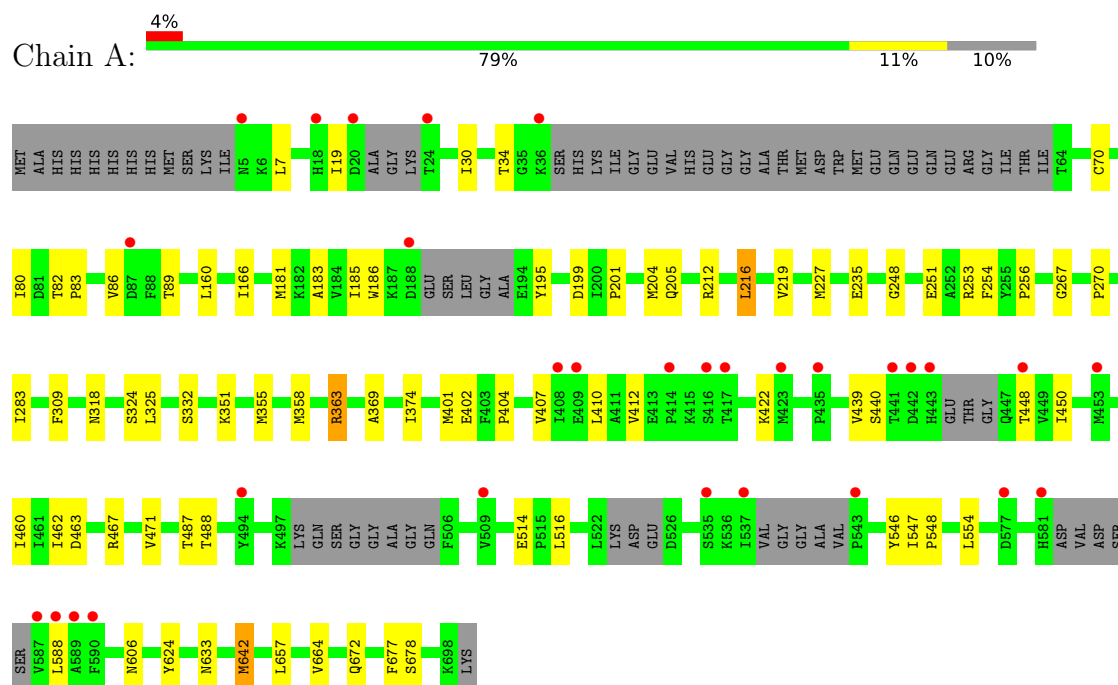
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	27	Total	O	0	0
			27	27		
2	B	11	Total	O	0	0
			11	11		

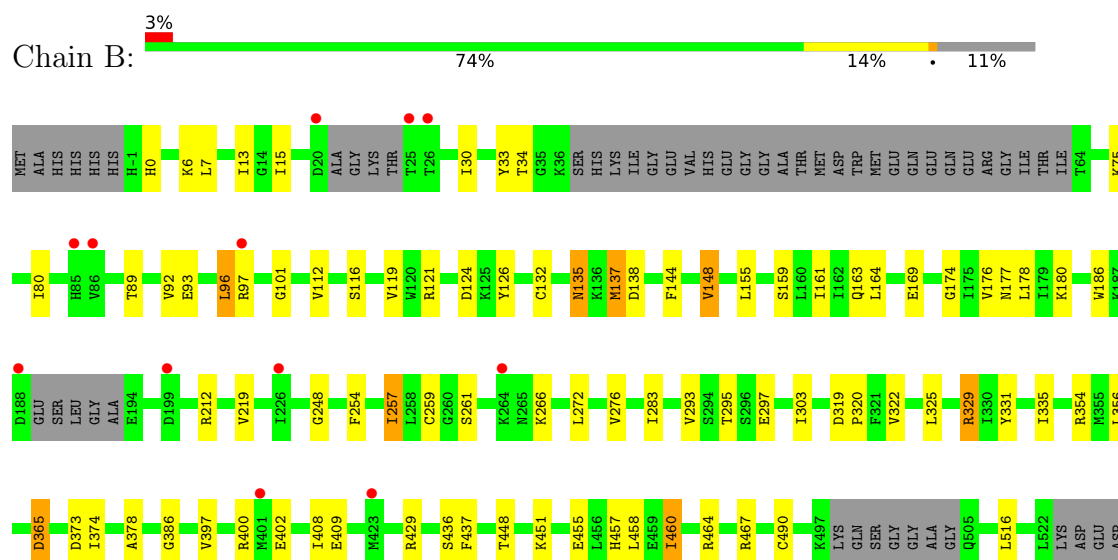
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Elongation factor G



• Molecule 1: Elongation factor G





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.67Å 79.56Å 95.47Å 103.85° 95.32° 92.17°	Depositor
Resolution (Å)	32.60 – 2.40 32.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (32.60-2.40) 98.2 (32.60-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.39Å)	Xtriage
Refinement program	PHENIX (dev_3374)	Depositor
R, R_{free}	0.197 , 0.244 0.200 , 0.244	Depositor DCC
R_{free} test set	3135 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9355	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/4749	0.43	0/6447
1	B	0.22	0/4711	0.42	0/6401
All	All	0.22	0/9460	0.42	0/12848

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4679	0	4435	38	0
1	B	4638	0	4424	56	0
2	A	27	0	0	0	0
2	B	11	0	0	3	0
All	All	9355	0	8859	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ILE:HD11	1:B:374:ILE:HD13	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ILE:HD11	1:A:374:ILE:HD13	1.61	0.80
1:B:409:GLU:HG2	1:B:451:LYS:HG2	1.67	0.76
1:B:354:ARG:NH2	1:B:365:ASP:OD2	2.19	0.75
1:B:93:GLU:OE2	1:B:126:TYR:OH	2.04	0.72
1:B:148:VAL:HG11	1:B:161:ILE:HD11	1.73	0.71
1:B:164:LEU:HG	1:B:178:LEU:HD11	1.77	0.66
1:A:624:TYR:OH	1:A:672:GLN:NE2	2.27	0.65
1:B:138:ASP:OD1	1:B:261:SER:OG	2.17	0.62
1:B:30:ILE:HG23	1:B:272:LEU:HD21	1.84	0.60
1:A:166:ILE:HA	1:A:204:MET:HE1	1.83	0.60
1:B:457:HIS:HA	1:B:460:ILE:HD12	1.84	0.60
1:A:89:THR:HG21	1:A:678:SER:HB3	1.83	0.59
1:B:137:MET:HE1	1:B:144:PHE:HB2	1.85	0.59
1:B:437:PHE:O	2:B:701:HOH:O	2.17	0.58
1:B:553:GLY:HA2	1:B:595:LYS:HE3	1.86	0.58
1:B:93:GLU:O	1:B:97[A]:ARG:HG2	2.05	0.57
1:A:407:VAL:HB	1:A:657:LEU:HD22	1.87	0.56
1:B:386:GLY:O	1:B:400:ARG:HD3	2.06	0.55
1:B:7:LEU:HD21	1:B:303:ILE:HG22	1.89	0.54
1:B:7:LEU:HG	1:B:283:ILE:HG13	1.90	0.53
1:B:354:ARG:HG3	1:B:378:ALA:HB3	1.91	0.53
1:B:622:ASP:OD2	1:B:622:ASP:N	2.39	0.53
1:B:563:ILE:HD11	1:B:607:PRO:HB2	1.91	0.52
1:A:422:LYS:HB3	1:A:471:VAL:HG22	1.90	0.52
1:B:176:VAL:HG12	1:B:178:LEU:HD12	1.92	0.52
1:A:34:THR:HG21	1:A:70:CYS:SG	2.49	0.51
1:B:436:SER:OG	1:B:457:HIS:NE2	2.41	0.51
1:B:30:ILE:O	1:B:34:THR:HG23	2.11	0.51
1:A:82:THR:N	1:A:83:PRO:HD2	2.27	0.50
1:B:13:ILE:HA	1:B:101:GLY:O	2.11	0.50
1:A:410:LEU:HD23	1:A:450:ILE:HD11	1.92	0.50
1:A:160:LEU:HD22	1:A:254:PHE:CE1	2.47	0.50
1:B:562:VAL:HG11	1:B:602:MET:HB2	1.93	0.50
1:B:112:VAL:HG11	1:B:155:LEU:HD21	1.94	0.49
1:A:251:GLU:OE2	1:A:253:ARG:NH1	2.46	0.49
1:B:132:CYS:HB2	1:B:257:ILE:HD13	1.95	0.48
1:A:160:LEU:O	1:A:256:PRO:HA	2.14	0.48
1:A:30:ILE:O	1:A:34:THR:HG23	2.13	0.48
1:B:354:ARG:HH21	1:B:365:ASP:CG	2.19	0.48
1:B:408:ILE:HG23	1:B:458:LEU:HD11	1.96	0.48
1:B:635:ARG:HB3	1:B:659:GLU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ASN:HD22	1:B:135:ASN:H	1.62	0.47
1:B:159:SER:HB3	1:B:257:ILE:HG13	1.96	0.47
1:B:248:GLY:HA3	1:B:254:PHE:CZ	2.50	0.47
1:A:309:PHE:HA	1:A:332:SER:O	2.15	0.46
1:A:186:TRP:CD1	1:A:195:TYR:HB3	2.51	0.46
1:A:546:TYR:HE2	1:A:588:LEU:HA	1.81	0.46
1:B:547:ILE:N	1:B:548:PRO:HD2	2.31	0.46
1:B:625:MET:HE1	1:B:642:MET:HG3	1.97	0.46
1:B:319:ASP:OD2	1:B:322:VAL:HG22	2.16	0.46
1:B:664:VAL:HG22	1:B:677:PHE:HE1	1.81	0.46
1:B:137:MET:CE	1:B:144:PHE:HB2	2.45	0.46
1:A:546:TYR:CE2	1:A:588:LEU:HA	2.52	0.45
1:A:516:LEU:HD23	1:A:516:LEU:HA	1.82	0.45
1:B:75:LYS:HE3	1:B:276:VAL:HG13	1.99	0.45
1:B:137:MET:HE2	1:B:259:CYS:HB2	1.99	0.45
1:A:402:GLU:O	1:A:404:PRO:HD3	2.17	0.45
1:B:177:ASN:CG	1:B:180:LYS:HG2	2.42	0.44
1:B:325:LEU:HD21	1:B:356:LEU:HD12	1.98	0.44
1:A:463:ASP:OD2	1:A:467:ARG:NE	2.50	0.44
1:A:181:MET:SD	1:A:212:ARG:HD3	2.58	0.44
1:B:329:ARG:HG2	1:B:331:TYR:CE2	2.53	0.44
1:B:96:LEU:O	2:B:702:HOH:O	2.21	0.43
1:B:516:LEU:HD23	1:B:516:LEU:HA	1.81	0.43
1:A:358:MET:HE3	1:A:363:ARG:HE	1.82	0.43
1:B:568:MET:HE2	1:B:568:MET:HB3	1.65	0.43
1:A:487:THR:HG22	1:A:488:THR:HG23	1.99	0.43
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.72	0.43
1:A:642:MET:HE2	1:A:642:MET:HB2	1.80	0.43
1:A:267:GLY:C	1:A:270:PRO:HD2	2.44	0.43
1:B:319:ASP:OD1	1:B:320:PRO:HD2	2.18	0.43
1:B:293:VAL:HG22	1:B:397:VAL:HG23	2.01	0.42
1:A:183:ALA:HB2	1:A:201:PRO:HD3	2.00	0.42
1:A:212:ARG:O	1:A:216:LEU:HD12	2.19	0.42
1:B:163:GLN:HA	1:B:176:VAL:O	2.19	0.42
1:B:295:THR:HG23	1:B:297:GLU:H	1.83	0.42
1:B:685:ASP:HB2	2:B:705:HOH:O	2.19	0.42
1:A:185:ILE:O	1:A:195:TYR:HB2	2.20	0.42
1:B:6:LYS:HE3	1:B:373:ASP:OD1	2.20	0.42
1:B:116:SER:HA	1:B:119:VAL:HG22	2.01	0.41
1:B:186:TRP:HB2	1:B:266:LYS:HD3	2.01	0.41
1:A:547:ILE:N	1:A:548:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:VAL:HB	1:A:448:THR:HG23	2.01	0.41
1:B:92:VAL:O	1:B:96:LEU:HB2	2.20	0.41
1:A:248:GLY:HA3	1:A:254:PHE:CZ	2.56	0.41
1:A:633:ASN:HD22	1:A:633:ASN:HA	1.72	0.41
1:A:487:THR:HB	1:A:606:ASN:HB2	2.02	0.41
1:A:554:LEU:HD23	1:A:554:LEU:HA	1.92	0.41
1:A:664:VAL:HG22	1:A:677:PHE:HE1	1.85	0.41
1:A:355:MET:HE1	1:A:369:ALA:HB3	2.03	0.40
1:B:464:ARG:HG3	1:B:467:ARG:NH2	2.35	0.40
1:A:7:LEU:HD23	1:A:283:ILE:HD11	2.03	0.40
1:B:174:GLY:HA2	1:B:186:TRP:CE3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	617/707 (87%)	586 (95%)	29 (5%)	2 (0%)	36	50
1	B	616/707 (87%)	593 (96%)	23 (4%)	0	100	100
All	All	1233/1414 (87%)	1179 (96%)	52 (4%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	VAL
1	A	19	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	460/599 (77%)	443 (96%)	17 (4%)	30	51
1	B	458/599 (76%)	429 (94%)	29 (6%)	16	29
All	All	918/1198 (77%)	872 (95%)	46 (5%)	22	38

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	ASP
1	A	205	GLN
1	A	216	LEU
1	A	219	VAL
1	A	227	MET
1	A	235	GLU
1	A	318	ASN
1	A	324	SER
1	A	351	LYS
1	A	363	ARG
1	A	401	MET
1	A	439	VAL
1	A	440	SER
1	A	460	ILE
1	A	462	ILE
1	A	514	GLU
1	A	642	MET
1	B	0	HIS
1	B	15	ILE
1	B	33	TYR
1	B	89	THR
1	B	96	LEU
1	B	121	ARG
1	B	124	ASP
1	B	135	ASN
1	B	137	MET
1	B	148	VAL

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Mol	Chain	Res	Type
1	B	169	GLU
1	B	212	ARG
1	B	219	VAL
1	B	257	ILE
1	B	329	ARG
1	B	335	ILE
1	B	365	ASP
1	B	402	GLU
1	B	429	ARG
1	B	448	THR
1	B	455	GLU
1	B	460	ILE
1	B	490	CYS
1	B	568	MET
1	B	592	ILE
1	B	599	ARG
1	B	622	ASP
1	B	676	GLN
1	B	694	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	229	GLN
1	A	318	ASN
1	A	496	HIS
1	A	633	ASN
1	A	654	HIS
1	A	672	GLN
1	B	135	ASN
1	B	318	ASN
1	B	362	ASN
1	B	420	GLN
1	B	649	GLN
1	B	672	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	635/707 (89%)	0.18	30 (4%) 36 32	47, 82, 143, 179	0
1	B	631/707 (89%)	0.17	19 (3%) 52 48	47, 84, 146, 187	1 (0%)
All	All	1266/1414 (89%)	0.18	49 (3%) 43 39	47, 83, 145, 187	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	546	TYR	4.7
1	A	188	ASP	4.5
1	B	226	ILE	3.3
1	A	18	HIS	3.3
1	A	537	ILE	3.3
1	A	587	VAL	3.1
1	A	435	PRO	3.0
1	A	416	SER	3.0
1	A	417	THR	3.0
1	B	199	ASP	2.9
1	B	423	MET	2.9
1	B	537	ILE	2.8
1	B	86	VAL	2.8
1	B	532	VAL	2.7
1	A	448	THR	2.7
1	B	25	THR	2.7
1	B	97[A]	ARG	2.7
1	A	590	PHE	2.7
1	B	264	LYS	2.6
1	B	401	MET	2.6
1	A	87	ASP	2.5
1	A	588	LEU	2.5
1	A	494	TYR	2.5
1	A	24	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	85	HIS	2.4
1	B	550	VAL	2.4
1	A	20	ASP	2.3
1	B	188	ASP	2.3
1	B	576	VAL	2.3
1	A	589	ALA	2.3
1	B	593	ALA	2.3
1	B	26	THR	2.3
1	A	423	MET	2.3
1	A	414	PRO	2.3
1	A	581	HIS	2.3
1	A	443	HIS	2.2
1	B	589	ALA	2.2
1	A	441	THR	2.2
1	B	20	ASP	2.2
1	A	36	LYS	2.2
1	A	408	ILE	2.2
1	A	409	GLU	2.2
1	A	577	ASP	2.1
1	A	509	VAL	2.1
1	A	535	SER	2.1
1	A	543	PRO	2.1
1	A	5	ASN	2.1
1	A	442	ASP	2.0
1	A	453	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.